Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 11:31 pm BST

PDB ID	:	2XJN
Title	:	Crystal structure of Streptococcus suis Dpr with copper
Authors	:	Haikarainen, T.; Thanassoulas, A.; Stavros, P.; Nounesis, G.; Haataja, S.; Papageorgiou, A.C.
Deposited on	:	2010-07-06
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

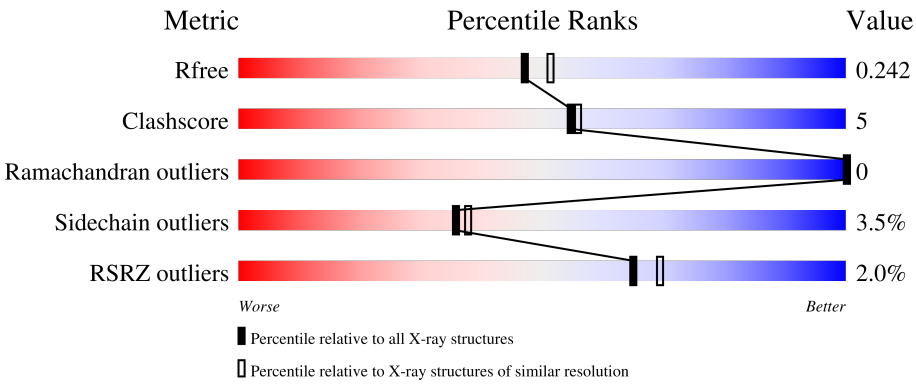
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	78% 12% • 9%
1	B	165	77% 13% • 8%
1	C	165	83% 6% • 10%
1	D	165	84% 7% • 8%
1	E	165	79% 13% 8%

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Mol	Chain	Length	Quality of chain
1	F	165	% 82% 9% • 8%
1	G	165	% 82% 8% • 8%
1	H	165	5% 82% 8% • 8%
1	I	165	2% 78% 13% • 8%
1	J	165	3% 82% 8% • 8%
1	K	165	% 80% 12% • 8%
1	L	165	% 77% 13% • 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA PROTECTION DURING STARVATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1213	771	200	236	6	0	2	0
1	B	151	1226	781	201	237	7	0	2	0
1	C	149	1212	771	202	233	6	0	2	0
1	D	151	1233	784	204	239	6	0	3	0
1	E	151	1221	777	200	238	6	0	3	0
1	F	151	1218	776	200	236	6	0	1	0
1	G	151	1233	783	205	238	7	0	3	0
1	H	151	1219	775	201	237	6	0	2	0
1	I	151	1220	777	200	237	6	0	2	0
1	J	151	1231	783	201	241	6	0	3	0
1	K	152	1238	787	202	243	6	0	3	0
1	L	151	1237	786	205	240	6	0	3	0

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

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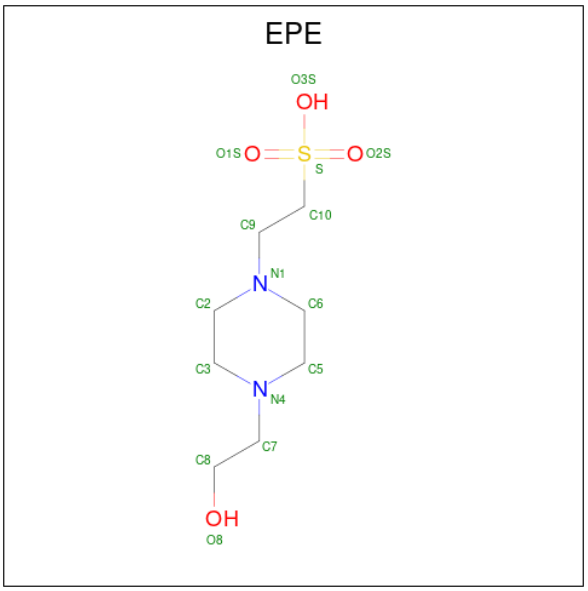
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0
2	I	1	1	1	0	0
2	J	1	1	1	0	0
2	K	1	1	1	0	0
2	L	1	1	1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
3	D	1	1	1	0	0
3	F	1	1	1	0	0
3	H	1	1	1	0	0
3	I	1	1	1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	15	8	2	4	1	0	0
4	E	1	15	8	2	4	1	0	0
4	I	1	15	8	2	4	1	0	0
4	K	1	15	8	2	4	1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	F	1	1	1	0	0
5	H	1	1	1	0	0
5	I	1	1	1	0	0
5	J	1	1	1	0	0
5	L	1	1	1	0	0

- Molecule 6 is water.

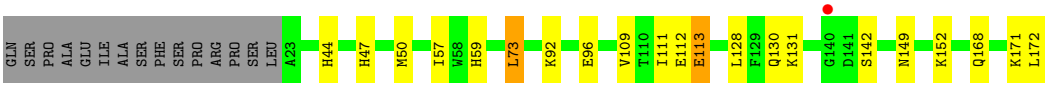
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	110	110	110	0	0
			Total	O		
6	B	122	122	122	0	0
			Total	O		
6	C	90	90	90	0	0
			Total	O		
6	D	129	129	129	0	0
			Total	O		
6	E	87	87	87	0	0
			Total	O		
6	F	107	107	107	0	0
			Total	O		
6	G	100	100	100	0	0
			Total	O		
6	H	92	92	92	0	0
			Total	O		
6	I	110	110	110	0	0
			Total	O		
6	J	90	90	90	0	0
			Total	O		
6	K	129	129	129	0	0
			Total	O		
6	L	91	91	91	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

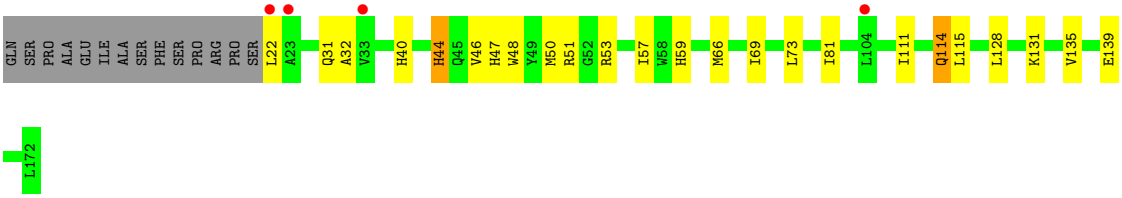
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain A: %
78% 12% • 9%



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain B: 2%
77% 13% • 8%



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

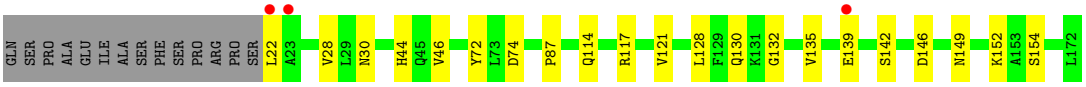
Chain C: 2%
83% 6% • 10%

• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain D: 2%
84% 7% • 8%

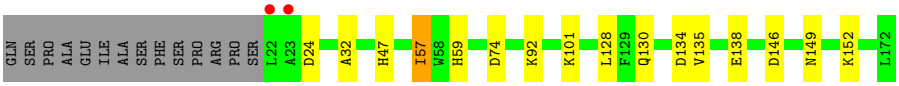
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain E: 2%
79% 13% 8%



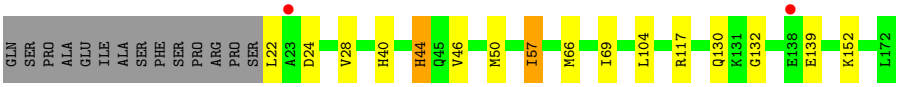
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain F:



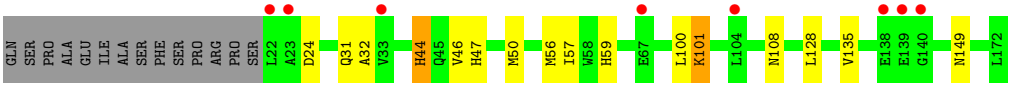
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain G:



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain H:

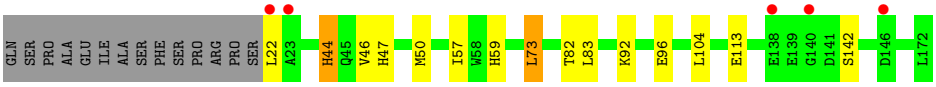


• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain I:

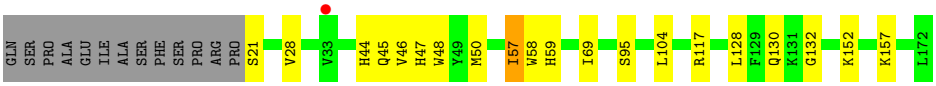
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain J:



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain K:



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain L:

GLN
SER
PRO
ALA
GLU
ILE
ALA
SER
PHE
SER
PRO
ARG
PRO
SER
L22
A23
D24
H40
H44
Q45
V46
H47
M50
R51
H59
E67
D74
L104
I111
Q114
R117
V118
V119
Q130
V135
E138
K152
I155
I159
W160
Q163
L172

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.84Å 137.71Å 142.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.76 – 2.10 24.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.76-2.10) 98.7 (24.76-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0078	Depositor
R, R_{free}	0.160 , 0.211 0.195 , 0.242	Depositor DCC
R_{free} test set	5932 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 29.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16040	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CA, EPE, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.69	0/1242	0.68	0/1677
1	B	0.71	0/1251	0.69	1/1688 (0.1%)
1	C	0.63	0/1237	0.64	1/1669 (0.1%)
1	D	0.78	1/1262 (0.1%)	0.69	1/1703 (0.1%)
1	E	0.62	0/1250	0.64	0/1689
1	F	0.71	0/1243	0.64	0/1678
1	G	0.64	0/1258	0.65	0/1697
1	H	0.63	0/1244	0.63	0/1680
1	I	0.76	1/1249 (0.1%)	0.68	0/1686
1	J	0.69	0/1260	0.66	1/1701 (0.1%)
1	K	0.73	0/1267	0.69	0/1710
1	L	0.66	0/1262	0.67	1/1703 (0.1%)
All	All	0.69	2/15025 (0.0%)	0.66	5/20281 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	GLU	CG-CD	5.45	1.60	1.51
1	I	120	GLU	CG-CD	5.04	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	73	LEU	CA-CB-CG	6.11	129.35	115.30
1	D	69	ILE	CG1-CB-CG2	-5.87	98.49	111.40
1	C	73	LEU	CA-CB-CG	5.72	128.47	115.30
1	B	73	LEU	CA-CB-CG	5.64	128.28	115.30
1	L	51	ARG	NE-CZ-NH2	-5.45	117.58	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1213	0	1168	18	0
1	B	1226	0	1187	22	0
1	C	1212	0	1171	7	0
1	D	1233	0	1191	13	0
1	E	1221	0	1170	13	0
1	F	1218	0	1179	13	0
1	G	1233	0	1188	14	0
1	H	1219	0	1169	17	0
1	I	1220	0	1180	13	0
1	J	1231	0	1184	16	0
1	K	1238	0	1191	15	0
1	L	1237	0	1194	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
4	B	15	0	17	1	0
4	E	15	0	17	0	0
4	I	15	0	17	0	0
4	K	15	0	17	0	0
5	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	A	110	0	0	2	0
6	B	122	0	0	0	0
6	C	90	0	0	1	0
6	D	129	0	0	3	0
6	E	87	0	0	2	0
6	F	107	0	0	1	0
6	G	100	0	0	4	0
6	H	92	0	0	2	0
6	I	110	0	0	3	0
6	J	90	0	0	2	0
6	K	129	0	0	2	0
6	L	91	0	0	0	0
All	All	16040	0	14240	150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ILE:HD11	1:J:57:ILE:HD11	1.26	1.17
1:L:117[A]:ARG:HG3	1:L:117[A]:ARG:HH21	1.00	1.15
1:B:57:ILE:HD11	1:J:57:ILE:CD1	1.80	1.09
1:D:117[B]:ARG:HH11	1:D:117[B]:ARG:HG3	1.14	1.07
1:A:57:ILE:HD11	1:H:57:ILE:HG13	1.05	1.04
1:G:40:HIS:HD2	6:G:2012:HOH:O	1.43	1.01
1:L:117[A]:ARG:HG3	1:L:117[A]:ARG:NH2	1.68	1.00
1:A:57:ILE:CD1	1:H:57:ILE:HG13	1.91	1.00
1:A:57:ILE:HD11	1:H:57:ILE:CG1	1.93	0.97
1:C:24:ASP:N	6:C:2001:HOH:O	2.00	0.95
1:G:130:GLN:HE21	1:G:152:LYS:HE3	1.33	0.93
1:D:117[B]:ARG:HG3	1:D:117[B]:ARG:NH1	1.77	0.91
1:G:117[B]:ARG:NH2	6:G:2070:HOH:O	2.05	0.89
1:G:130:GLN:NE2	1:G:152:LYS:HE3	1.87	0.89
1:L:130:GLN:HE21	1:L:152:LYS:HE3	1.35	0.88
1:B:40:HIS:CE1	1:B:66[B]:MET:HE3	2.12	0.84
1:F:130:GLN:NE2	1:F:152:LYS:HE3	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117[A]:ARG:HH21	1:L:117[A]:ARG:CG	1.86	0.84
1:D:117[B]:ARG:HH11	1:D:117[B]:ARG:CG	1.91	0.81
1:A:130:GLN:HE21	1:A:152:LYS:HE3	1.47	0.79
1:L:130:GLN:NE2	1:L:152:LYS:HE3	1.98	0.78
1:H:57:ILE:HD11	1:K:57:ILE:HG21	1.66	0.76
1:K:117:ARG:HD3	6:K:2089:HOH:O	1.86	0.75
1:E:152:LYS:HE3	6:E:2069:HOH:O	1.87	0.73
1:F:134:ASP:O	1:F:138:GLU:HG3	1.89	0.72
1:J:113:GLU:OE2	6:J:2063:HOH:O	2.08	0.71
1:J:92:LYS:O	1:J:96:GLU:HG3	1.91	0.70
1:B:40:HIS:CE1	1:B:66[B]:MET:CE	2.75	0.69
1:A:130:GLN:NE2	1:A:152:LYS:HE3	2.08	0.68
1:B:114:GLN:HE21	1:B:114:GLN:HA	1.61	0.65
1:F:130:GLN:HE21	1:F:152:LYS:HE3	1.60	0.65
1:A:112:GLU:HG3	6:A:2080:HOH:O	1.94	0.65
1:L:45:GLN:HE21	1:L:117[B]:ARG:HH22	1.45	0.65
1:A:57:ILE:HG12	1:K:57:ILE:CG2	2.27	0.64
1:I:40:HIS:CD2	1:I:70:ASP:OD2	2.54	0.61
1:D:56:MET:CG	1:G:57:ILE:HD11	2.31	0.59
1:F:24:ASP:HB3	1:F:135:VAL:CG1	2.33	0.58
1:G:24:ASP:HB2	1:G:139:GLU:OE1	2.04	0.56
1:E:74:ASP:OD2	1:G:44:HIS:HE1	1.90	0.55
1:B:22:LEU:HD21	1:B:31:GLN:HE21	1.72	0.55
1:H:24:ASP:HB3	1:H:135:VAL:HG13	1.89	0.55
1:A:92:LYS:O	1:A:96:GLU:HG2	2.06	0.55
1:C:172:LEU:HD11	1:J:82:THR:HG22	1.89	0.55
1:H:24:ASP:HB3	1:H:135:VAL:CG1	2.37	0.55
1:H:108:ASN:O	6:H:2059:HOH:O	2.18	0.55
1:I:44:HIS:HD2	6:I:2012:HOH:O	1.89	0.55
1:G:40:HIS:CD2	6:G:2012:HOH:O	2.31	0.54
1:B:50:MET:HG3	1:B:111:ILE:HD13	1.90	0.54
1:B:57:ILE:CD1	1:J:57:ILE:CD1	2.71	0.54
1:E:117:ARG:HG3	1:E:117:ARG:HH11	1.73	0.54
1:B:57:ILE:HD11	1:J:57:ILE:CG1	2.37	0.53
1:F:24:ASP:HB3	1:F:135:VAL:HG11	1.90	0.53
1:C:142:SER:OG	1:H:149:ASN:ND2	2.42	0.52
1:G:57:ILE:C	1:G:57:ILE:HD13	2.29	0.52
1:C:47:HIS:CE1	1:C:59:HIS:CE1	2.97	0.52
1:E:135:VAL:O	1:E:139:GLU:HG2	2.10	0.52
1:G:28:VAL:HG11	1:G:132:GLY:HA2	1.93	0.51
1:H:57:ILE:HD13	1:H:57:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ILE:CD1	1:J:57:ILE:HG13	2.40	0.51
1:E:130:GLN:HE21	1:E:152:LYS:HE3	1.75	0.51
1:L:50:MET:HG3	1:L:111:ILE:HD13	1.93	0.51
1:J:46:VAL:O	1:J:50:MET:HB2	2.12	0.50
1:D:56:MET:HG2	1:G:57:ILE:HD11	1.92	0.50
1:E:142:SER:OG	1:I:149:ASN:ND2	2.45	0.50
1:D:157:LYS:HE3	6:D:2121:HOH:O	2.11	0.50
1:A:168:GLN:HE21	1:A:171:LYS:NZ	2.09	0.50
1:I:72:TYR:OH	1:I:154[B]:SER:OG	2.26	0.50
1:J:22:LEU:HD12	1:J:83:LEU:HD22	1.92	0.49
1:L:24:ASP:HB2	1:L:135:VAL:HG13	1.94	0.49
1:I:47:HIS:CE1	1:I:59:HIS:CE1	3.01	0.49
1:B:135:VAL:O	1:B:139:GLU:HG3	2.13	0.49
1:I:40:HIS:HD2	1:I:70:ASP:OD2	1.93	0.49
1:A:113:GLU:HG3	6:A:2083:HOH:O	2.13	0.49
1:J:44:HIS:HE1	1:L:74:ASP:OD2	1.96	0.48
1:E:28:VAL:HG11	1:E:132:GLY:HA2	1.95	0.48
1:H:57:ILE:HD11	1:K:57:ILE:CG2	2.39	0.48
1:L:45:GLN:NE2	1:L:117[B]:ARG:HH12	2.11	0.48
1:A:50:MET:HG3	1:A:111:ILE:HD13	1.95	0.47
1:I:26:LYS:NZ	6:I:2003:HOH:O	2.45	0.47
1:E:152:LYS:CE	6:E:2069:HOH:O	2.56	0.47
1:K:57:ILE:HD11	1:K:58:TRP:CE2	2.50	0.47
1:I:112:GLU:HG3	6:I:2077:HOH:O	2.13	0.47
1:K:130:GLN:NE2	1:K:152:LYS:HE3	2.29	0.47
1:H:100:LEU:C	1:H:101:LYS:HD2	2.35	0.47
1:B:44:HIS:HE1	1:D:74:ASP:OD2	1.98	0.47
1:J:47:HIS:CE1	1:J:59:HIS:CE1	3.04	0.46
1:D:46:VAL:O	1:D:50:MET:HB2	2.15	0.46
1:I:81:ILE:HD11	1:K:48:TRP:HB3	1.98	0.46
1:L:117[A]:ARG:NH2	1:L:117[A]:ARG:CG	2.51	0.46
1:F:146:ASP:OD1	6:F:2085:HOH:O	2.21	0.46
1:H:31:GLN:NE2	6:H:2003:HOH:O	2.48	0.46
1:L:67:GLU:HA	1:L:67:GLU:OE2	2.16	0.45
1:B:57:ILE:HD13	1:J:57:ILE:HG13	1.98	0.45
1:K:57:ILE:HD11	1:K:58:TRP:NE1	2.30	0.45
1:B:46:VAL:HG13	1:B:114:GLN:HB3	1.99	0.45
1:E:72:TYR:HH	1:E:154[B]:SER:HG	1.59	0.45
1:L:46:VAL:HG13	1:L:114:GLN:HB3	1.99	0.45
1:F:24:ASP:HB3	1:F:135:VAL:HG13	1.98	0.45
1:H:46:VAL:O	1:H:50:MET:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LEU:HA	6:D:2001:HOH:O	2.17	0.45
1:G:66[B]:MET:HB3	1:G:66[B]:MET:HE2	1.71	0.44
1:L:46:VAL:O	1:L:50:MET:HB2	2.17	0.44
1:F:74:ASP:OD2	1:H:44:HIS:HE1	1.99	0.44
1:G:22:LEU:N	6:G:2001:HOH:O	2.49	0.44
1:A:73:LEU:HD12	1:A:73:LEU:O	2.18	0.44
1:L:119:VAL:HG21	1:L:163:GLN:HE21	1.83	0.44
1:B:53:ARG:HB3	4:B:1173:EPE:H21	2.00	0.44
1:I:22:LEU:HD12	1:I:139:GLU:HB3	2.00	0.44
1:A:109:VAL:HG13	1:A:113:GLU:HB3	2.00	0.44
1:K:46:VAL:O	1:K:50:MET:HB2	2.17	0.44
1:B:57:ILE:CD1	1:J:57:ILE:CG1	2.95	0.44
1:D:22:LEU:N	6:D:2001:HOH:O	2.50	0.44
1:K:28:VAL:HG11	1:K:132:GLY:HA2	2.01	0.43
1:A:149:ASN:ND2	1:I:142:SER:OG	2.50	0.43
1:A:172:LEU:HD11	1:I:82:THR:HG22	2.00	0.43
1:F:47:HIS:CE1	1:F:59:HIS:CE1	3.06	0.43
1:L:24:ASP:CB	1:L:135:VAL:HG13	2.48	0.43
1:D:142:SER:OG	1:F:149:ASN:ND2	2.52	0.43
1:L:45:GLN:HE21	1:L:117[B]:ARG:NH2	2.15	0.43
1:B:51:ARG:O	1:B:111:ILE:HG12	2.19	0.43
1:F:32:ALA:HA	1:F:128:LEU:HD21	2.01	0.42
1:B:32:ALA:HA	1:B:128:LEU:HD21	2.00	0.42
1:C:101:LYS:HA	1:C:101:LYS:HD2	1.61	0.42
1:H:47:HIS:CE1	1:H:59:HIS:CE1	3.07	0.42
1:K:45:GLN:OE1	1:K:117:ARG:NH2	2.51	0.42
1:K:117:ARG:CD	6:K:2089:HOH:O	2.57	0.42
1:C:149:ASN:ND2	1:J:142:SER:OG	2.53	0.42
1:L:47:HIS:CE1	1:L:59:HIS:CE1	3.08	0.42
1:L:155:ILE:O	1:L:159:ILE:HG13	2.20	0.42
1:F:57:ILE:HD12	1:F:57:ILE:HG23	1.78	0.42
1:L:40:HIS:CD2	1:L:40:HIS:C	2.93	0.42
1:E:46:VAL:HG13	1:E:114:GLN:HB3	2.02	0.41
1:B:48:TRP:HB3	1:D:81:ILE:HD11	2.01	0.41
1:B:81:ILE:HD11	1:D:48:TRP:HB3	2.02	0.41
1:E:117:ARG:O	1:E:121:VAL:HG23	2.21	0.41
1:B:47:HIS:CE1	1:B:59:HIS:CE1	3.08	0.41
1:L:50:MET:CG	1:L:111:ILE:HD13	2.50	0.41
1:B:40:HIS:CE1	1:B:66[B]:MET:HE1	2.55	0.41
1:C:155:ILE:O	1:C:159:ILE:HG13	2.20	0.41
1:A:142:SER:OG	1:E:149:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:LEU:HA	1:I:139:GLU:OE1	2.21	0.41
1:A:47:HIS:CE1	1:A:59:HIS:CE1	3.08	0.41
1:F:57:ILE:HG13	1:J:57:ILE:HD11	2.03	0.41
1:G:46:VAL:O	1:G:50:MET:HB2	2.21	0.41
1:H:32:ALA:HA	1:H:128:LEU:HD21	2.03	0.41
1:H:56:MET:HB3	1:K:57:ILE:HD13	2.03	0.41
1:E:30:ASN:OD1	1:E:87:PRO:HA	2.21	0.40
6:J:2006:HOH:O	1:L:44:HIS:HD2	2.05	0.40
1:A:57:ILE:HG12	1:K:57:ILE:HG22	2.01	0.40
1:K:47:HIS:CE1	1:K:59:HIS:CE1	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	B	151/165 (92%)	149 (99%)	2 (1%)	0	100	100
1	C	149/165 (90%)	148 (99%)	1 (1%)	0	100	100
1	D	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	E	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	F	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	G	152/165 (92%)	150 (99%)	2 (1%)	0	100	100
1	H	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	I	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	J	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	K	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
1	L	152/165 (92%)	151 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1815/1980 (92%)	1801 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/141 (92%)	125 (96%)	5 (4%)	33	34
1	B	131/141 (93%)	126 (96%)	5 (4%)	33	34
1	C	129/141 (92%)	125 (97%)	4 (3%)	40	43
1	D	132/141 (94%)	129 (98%)	3 (2%)	50	55
1	E	130/141 (92%)	126 (97%)	4 (3%)	40	43
1	F	130/141 (92%)	127 (98%)	3 (2%)	50	55
1	G	131/141 (93%)	127 (97%)	4 (3%)	40	43
1	H	129/141 (92%)	127 (98%)	2 (2%)	62	69
1	I	131/141 (93%)	122 (93%)	9 (7%)	15	12
1	J	132/141 (94%)	129 (98%)	3 (2%)	50	55
1	K	133/141 (94%)	125 (94%)	8 (6%)	19	16
1	L	132/141 (94%)	126 (96%)	6 (4%)	27	27
All	All	1570/1692 (93%)	1514 (96%)	56 (4%)	36	36

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	73	LEU
1	A	113	GLU
1	A	128	LEU
1	A	131	LYS
1	B	44	HIS

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Mol	Chain	Res	Type
1	B	69	ILE
1	B	114	GLN
1	B	115	LEU
1	B	131	LYS
1	C	44	HIS
1	C	69	ILE
1	C	73	LEU
1	C	101	LYS
1	D	44	HIS
1	D	117[A]	ARG
1	D	117[B]	ARG
1	E	22	LEU
1	E	44	HIS
1	E	128	LEU
1	E	146	ASP
1	F	57	ILE
1	F	92	LYS
1	F	101	LYS
1	G	44	HIS
1	G	57	ILE
1	G	69	ILE
1	G	104	LEU
1	H	44	HIS
1	H	101	LYS
1	I	22	LEU
1	I	44	HIS
1	I	73	LEU
1	I	95	SER
1	I	99	GLN
1	I	104	LEU
1	I	128	LEU
1	I	138	GLU
1	I	146	ASP
1	J	44	HIS
1	J	73	LEU
1	J	104	LEU
1	K	21	SER
1	K	44	HIS
1	K	57	ILE
1	K	69	ILE
1	K	95	SER
1	K	104	LEU

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Mol	Chain	Res	Type
1	K	128	LEU
1	K	157	LYS
1	L	44	HIS
1	L	104	LEU
1	L	117[A]	ARG
1	L	117[B]	ARG
1	L	138	GLU
1	L	160	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	130	GLN
1	A	149	ASN
1	A	163	GLN
1	A	168	GLN
1	B	31	GLN
1	B	40	HIS
1	B	44	HIS
1	B	99	GLN
1	B	114	GLN
1	B	130	GLN
1	B	149	ASN
1	B	163	GLN
1	C	44	HIS
1	C	149	ASN
1	C	163	GLN
1	D	31	GLN
1	D	44	HIS
1	D	130	GLN
1	D	149	ASN
1	D	163	GLN
1	E	31	GLN
1	E	44	HIS
1	E	45	GLN
1	E	130	GLN
1	E	149	ASN
1	F	31	GLN
1	F	130	GLN
1	F	145	ASN
1	F	149	ASN

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Mol	Chain	Res	Type
1	F	163	GLN
1	G	31	GLN
1	G	40	HIS
1	G	44	HIS
1	G	130	GLN
1	G	149	ASN
1	G	163	GLN
1	H	31	GLN
1	H	40	HIS
1	H	44	HIS
1	H	45	GLN
1	H	99	GLN
1	H	149	ASN
1	I	40	HIS
1	I	44	HIS
1	I	99	GLN
1	I	145	ASN
1	I	149	ASN
1	I	163	GLN
1	J	44	HIS
1	J	130	GLN
1	J	149	ASN
1	K	31	GLN
1	K	44	HIS
1	K	99	GLN
1	K	130	GLN
1	K	149	ASN
1	L	44	HIS
1	L	45	GLN
1	L	130	GLN
1	L	149	ASN
1	L	163	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 22 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EPE	E	1173	-	15,15,15	1.08	1 (6%)	18,20,20	2.05	4 (22%)
4	EPE	K	1173	-	15,15,15	1.27	1 (6%)	18,20,20	2.87	6 (33%)
4	EPE	B	1173	-	15,15,15	0.90	1 (6%)	18,20,20	2.58	6 (33%)
4	EPE	I	1173	-	15,15,15	0.92	1 (6%)	18,20,20	2.31	8 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	E	1173	-	-	6/9/19/19	0/1/1/1
4	EPE	K	1173	-	-	4/9/19/19	0/1/1/1
4	EPE	B	1173	-	-	1/9/19/19	0/1/1/1
4	EPE	I	1173	-	-	2/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1173	EPE	C10-S	4.42	1.83	1.77
4	E	1173	EPE	C10-S	3.71	1.82	1.77
4	I	1173	EPE	C10-S	2.73	1.81	1.77
4	B	1173	EPE	C10-S	2.61	1.81	1.77

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1173	EPE	O1S-S-C10	8.42	117.06	106.92
4	E	1173	EPE	O1S-S-C10	5.43	113.45	106.92
4	B	1173	EPE	O2S-S-C10	-5.42	100.39	106.92
4	I	1173	EPE	C5-N4-C3	5.42	121.02	108.83
4	B	1173	EPE	O3S-S-C10	4.89	113.67	105.77
4	K	1173	EPE	C5-N4-C3	4.88	119.82	108.83
4	E	1173	EPE	C5-N4-C3	4.83	119.71	108.83
4	B	1173	EPE	C5-N4-C3	4.49	118.94	108.83
4	I	1173	EPE	O3S-S-C10	3.86	112.01	105.77
4	B	1173	EPE	C7-N4-C5	3.70	120.69	111.23
4	B	1173	EPE	O1S-S-C10	3.63	111.29	106.92
4	K	1173	EPE	C7-N4-C3	3.50	120.19	111.23
4	I	1173	EPE	C2-C3-N4	3.30	117.42	110.64
4	K	1173	EPE	O2S-S-C10	-3.07	103.22	106.92
4	K	1173	EPE	C7-N4-C5	3.07	119.08	111.23
4	I	1173	EPE	O1S-S-C10	3.03	110.57	106.92
4	K	1173	EPE	C3-C2-N1	-2.67	105.17	110.64
4	E	1173	EPE	C7-N4-C5	2.57	117.82	111.23
4	I	1173	EPE	C9-N1-C2	-2.48	104.90	111.23
4	E	1173	EPE	C7-N4-C3	2.39	117.35	111.23
4	B	1173	EPE	C7-N4-C3	2.39	117.35	111.23
4	I	1173	EPE	C6-C5-N4	2.36	115.48	110.64
4	I	1173	EPE	O2S-S-C10	-2.33	104.11	106.92
4	I	1173	EPE	C7-N4-C3	2.11	116.63	111.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1173	EPE	C8-C7-N4-C5
4	K	1173	EPE	C9-C10-S-O2S
4	E	1173	EPE	N4-C7-C8-O8
4	K	1173	EPE	C8-C7-N4-C5
4	E	1173	EPE	C9-C10-S-O3S
4	E	1173	EPE	C10-C9-N1-C6
4	K	1173	EPE	C9-C10-S-O3S
4	I	1173	EPE	C8-C7-N4-C5
4	E	1173	EPE	C9-C10-S-O1S
4	E	1173	EPE	C9-C10-S-O2S
4	K	1173	EPE	C9-C10-S-O1S
4	E	1173	EPE	C8-C7-N4-C5
4	I	1173	EPE	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1173	EPE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	150/165 (90%)	0.10	1 (0%)	87	89	21, 28, 38, 46	0
1	B	151/165 (91%)	0.10	4 (2%)	56	61	18, 24, 39, 71	0
1	C	149/165 (90%)	0.19	3 (2%)	65	69	25, 31, 45, 51	0
1	D	151/165 (91%)	0.04	3 (1%)	65	69	18, 23, 33, 41	0
1	E	151/165 (91%)	0.21	3 (1%)	65	69	27, 33, 49, 74	0
1	F	151/165 (91%)	0.15	2 (1%)	77	80	19, 25, 39, 53	0
1	G	151/165 (91%)	0.11	2 (1%)	77	80	23, 30, 45, 73	0
1	H	151/165 (91%)	0.21	8 (5%)	26	32	22, 30, 48, 57	0
1	I	151/165 (91%)	0.11	3 (1%)	65	69	18, 28, 44, 56	0
1	J	151/165 (91%)	0.11	5 (3%)	46	53	21, 31, 46, 65	0
1	K	152/165 (92%)	-0.00	1 (0%)	87	89	19, 25, 37, 47	0
1	L	151/165 (91%)	0.07	2 (1%)	77	80	22, 31, 45, 52	0
All	All	1810/1980 (91%)	0.12	37 (2%)	65	69	18, 29, 45, 74	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	22	LEU	4.7
1	H	22	LEU	4.5
1	H	23	ALA	4.5
1	F	23	ALA	4.4
1	G	23	ALA	4.1
1	I	23	ALA	4.0
1	B	23	ALA	3.8
1	E	23	ALA	3.6
1	F	22	LEU	3.3
1	A	140	GLY	3.2
1	J	22	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	139	GLU	2.8
1	E	22	LEU	2.7
1	D	22	LEU	2.7
1	B	22	LEU	2.5
1	H	104	LEU	2.4
1	L	22	LEU	2.4
1	J	23	ALA	2.4
1	J	138	GLU	2.4
1	B	104	LEU	2.3
1	C	67	GLU	2.3
1	G	138	GLU	2.3
1	J	140	GLY	2.3
1	H	67	GLU	2.3
1	D	33	VAL	2.3
1	L	138	GLU	2.3
1	B	33	VAL	2.3
1	H	138	GLU	2.2
1	C	131	LYS	2.2
1	D	23	ALA	2.2
1	H	139	GLU	2.2
1	C	99	GLN	2.1
1	H	33	VAL	2.1
1	J	146[A]	ASP	2.1
1	I	131	LYS	2.1
1	H	140	GLY	2.0
1	K	33	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	J	1174	1/1	0.94	0.27	30,30,30,30	0
4	EPE	E	1173	15/15	0.95	0.24	13,21,28,29	0
5	CA	I	1176	1/1	0.95	0.25	26,26,26,26	0
4	EPE	B	1173	15/15	0.95	0.17	15,23,30,31	0
4	EPE	I	1173	15/15	0.96	0.17	12,18,27,28	0
4	EPE	K	1173	15/15	0.96	0.16	13,20,22,23	0
5	CA	L	1174	1/1	0.96	0.27	24,24,24,24	0
5	CA	F	1174	1/1	0.97	0.15	12,12,12,12	0
5	CA	H	1175	1/1	0.97	0.17	29,29,29,29	0
3	CL	A	1174	1/1	0.97	0.22	19,19,19,19	0
3	CL	I	1175	1/1	0.97	0.20	22,22,22,22	0
2	CU	C	1173	1/1	0.97	0.10	16,16,16,16	1
2	CU	E	1174	1/1	0.98	0.11	16,16,16,16	1
3	CL	F	1175	1/1	0.98	0.23	22,22,22,22	0
2	CU	H	1173	1/1	0.98	0.07	16,16,16,16	1
2	CU	L	1173	1/1	0.98	0.08	16,16,16,16	1
2	CU	G	1173	1/1	0.99	0.10	18,18,18,18	1
2	CU	A	1173	1/1	0.99	0.18	10,10,10,10	1
2	CU	I	1174	1/1	0.99	0.05	17,17,17,17	1
2	CU	J	1173	1/1	0.99	0.15	13,13,13,13	1
2	CU	K	1174	1/1	0.99	0.05	15,15,15,15	1
2	CU	D	1173	1/1	0.99	0.04	16,16,16,16	1
2	CU	B	1174	1/1	0.99	0.04	16,16,16,16	1
3	CL	D	1174	1/1	0.99	0.16	20,20,20,20	0
2	CU	F	1173	1/1	0.99	0.16	7,7,7,7	1
3	CL	H	1174	1/1	0.99	0.22	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.